

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 298 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 3.26e-01

**Confidence level:** 4.78e-01

## Nearest Neighbors from the Training Set

Image not found

N-Butylbenzenesulfonamide

**Measured:** 314

**Predicted:** 286

Image not found

Ethyl oxanilate

**Measured:** 280

**Predicted:** 295

Image not found

Carbaryl

**Measured:** 315

**Predicted:** 297

Image not found

Phenacetin

**Measured:** 244

**Predicted:** 301

Image not found

2-Benzoxazolinone

**Measured:** 335

**Predicted:** 306